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## Typical Product Specifications & Properties

# DI Normetanephine

CAS Number: : 97-31-4

Specifications	Limits
SMILES	<chem>COc1cc(ccc1O)C(O)CN</chem>
InChI	YNYAYWLBAHXHLL-UHFFFAOYSA-N
InChIKey	1S/C9H13NO3/c1-13-9-4-6(8(12)5-10)2-3-7(9)11/h2-4,8,11-12H,5,10H2,1H3
Water solubility	1.00E+06 mg/L
Henry's Law Constant	1.83E-16 atm-m <sup>3</sup> /mole
Vapor Pressure	2.36E-06 mm Hg
log P (octanol-water)	-1.05E+00
Atmospheric OH Rate Constant	7.63E-11 cm <sup>3</sup> /molecule-sec
pKa Dissociation Constant	8.82



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